



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 09:15 pm BST

PDB ID : 6UJU
Title : Structure of the HIV-1 gp41 transmembrane domain and cytoplasmic tail (LLP2)
Authors : Piai, A.; Fu, Q.; Cai, Y.; Ghantous, F.; Xiao, T.; Shaik, M.M.; Peng, H.; Rits-Volloch, S.; Liu, Z.; Chen, W.; Seaman, M.S.; Chen, B.; Chou, J.J.
Deposited on : 2019-10-03

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

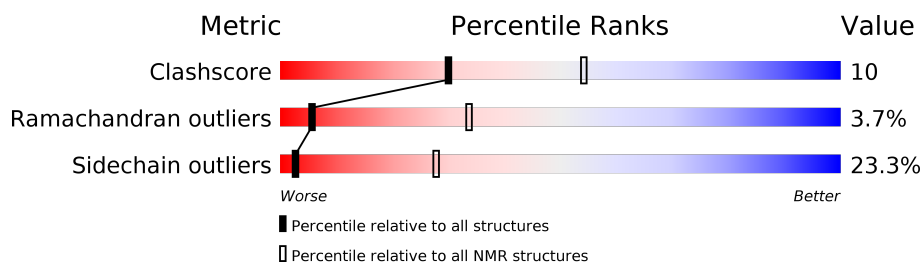
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 10%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	112	 50% 29% • 20%
1	B	112	 49% 30% • 20%
1	C	112	 46% 34% • 20%

2 Ensemble composition and analysis

This entry contains 15 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:679-A:716, A:739-A:788, B:677-B:716, B:739-B:788, C:677-C:716, C:739-C:788 (268)	1.00	13

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 5, 6, 8, 11, 12, 15
2	2, 3, 4, 7, 13
3	9, 14
Single-model clusters	10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4686 atoms, of which 2427 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope glycoprotein GP41.

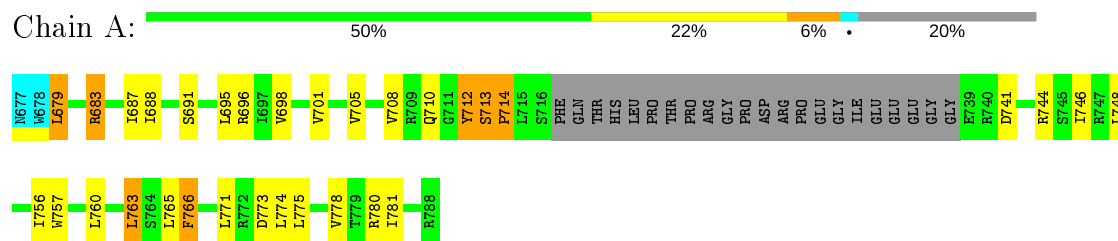
Mol	Chain	Residues	Atoms					Trace
1	A	90	Total	C	H	N	O	0
			1562	490	809	141	122	
1	B	90	Total	C	H	N	O	0
			1562	490	809	141	122	
1	C	90	Total	C	H	N	O	0
			1562	490	809	141	122	

There are 18 discrepancies between the modelled and reference sequences:

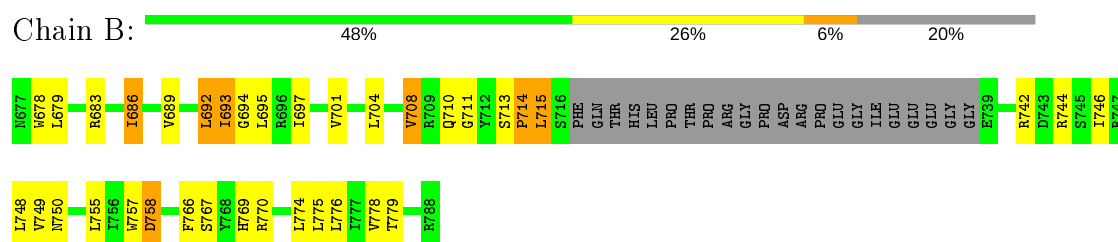
Chain	Residue	Modelled	Actual	Comment	Reference
A	683	ARG	LYS	conflict	UNP A0A386YSI0
A	687	ILE	MET	conflict	UNP A0A386YSI0
A	691	SER	GLY	conflict	UNP A0A386YSI0
A	693	ILE	VAL	conflict	UNP A0A386YSI0
A	704	LEU	ILE	conflict	UNP A0A386YSI0
A	764	SER	CYS	engineered mutation	UNP A0A386YSI0
B	683	ARG	LYS	conflict	UNP A0A386YSI0
B	687	ILE	MET	conflict	UNP A0A386YSI0
B	691	SER	GLY	conflict	UNP A0A386YSI0
B	693	ILE	VAL	conflict	UNP A0A386YSI0
B	704	LEU	ILE	conflict	UNP A0A386YSI0
B	764	SER	CYS	engineered mutation	UNP A0A386YSI0
C	683	ARG	LYS	conflict	UNP A0A386YSI0
C	687	ILE	MET	conflict	UNP A0A386YSI0
C	691	SER	GLY	conflict	UNP A0A386YSI0
C	693	ILE	VAL	conflict	UNP A0A386YSI0
C	704	LEU	ILE	conflict	UNP A0A386YSI0
C	764	SER	CYS	engineered mutation	UNP A0A386YSI0

4.2.1 Score per residue for model 1

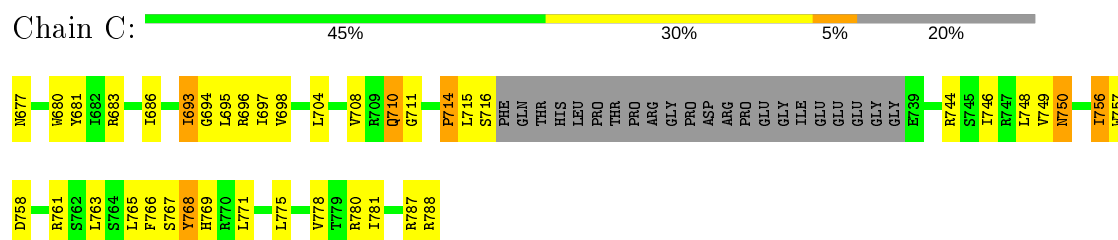
- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41

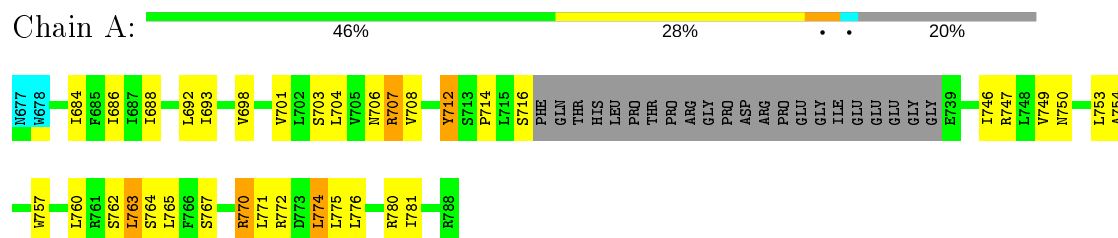


- Molecule 1: Envelope glycoprotein GP41



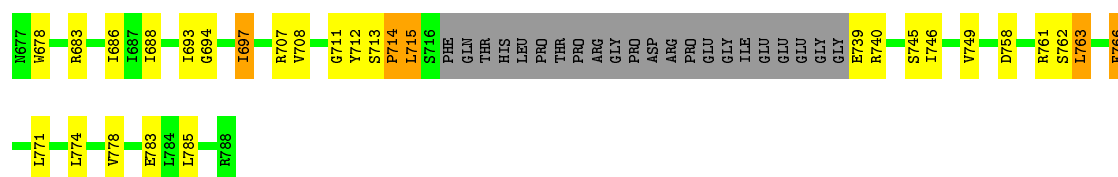
4.2.2 Score per residue for model 2

- Molecule 1: Envelope glycoprotein GP41

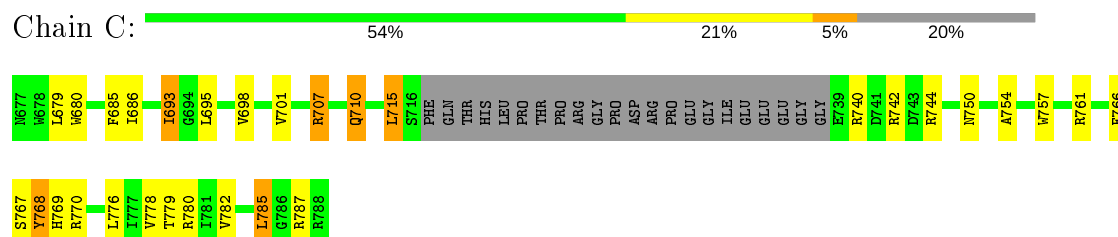


- Molecule 1: Envelope glycoprotein GP41



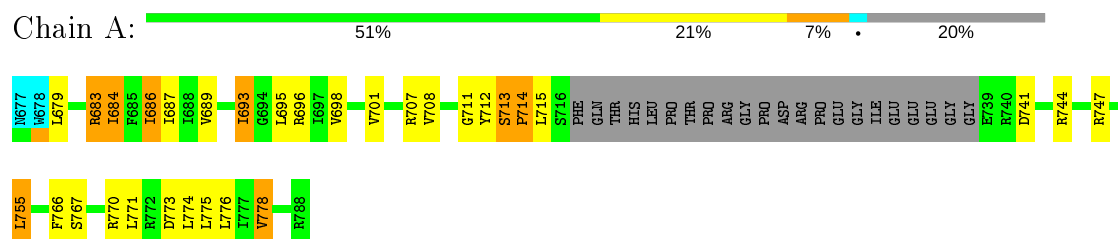


- Molecule 1: Envelope glycoprotein GP41

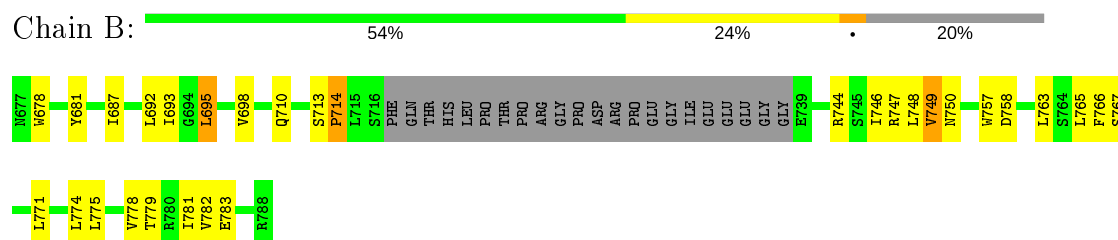


4.2.3 Score per residue for model 3

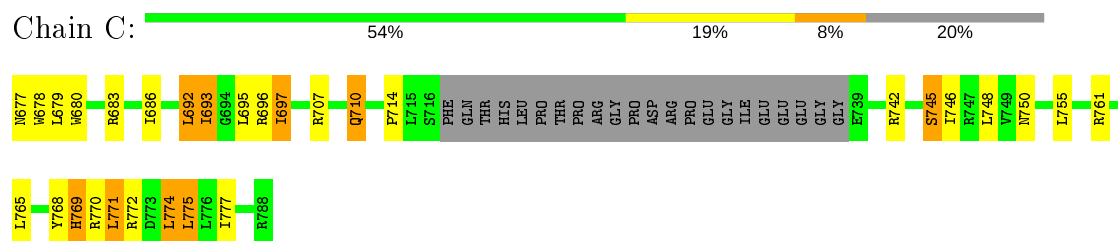
- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41

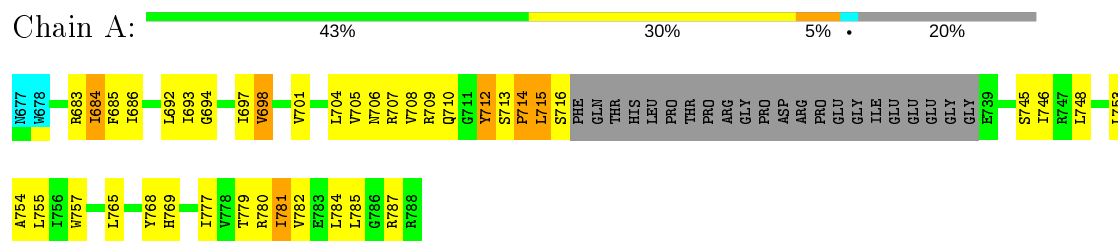


- Molecule 1: Envelope glycoprotein GP41

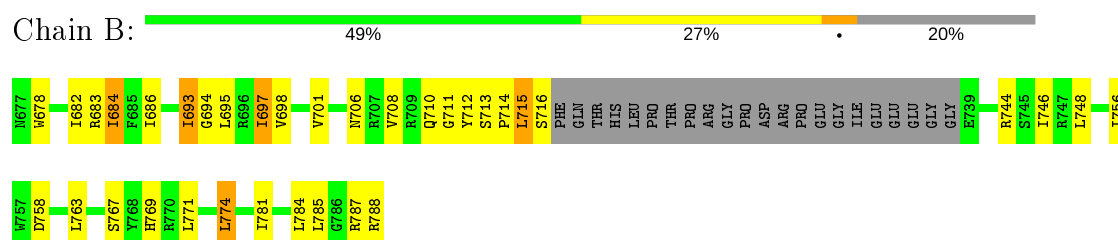


4.2.4 Score per residue for model 4

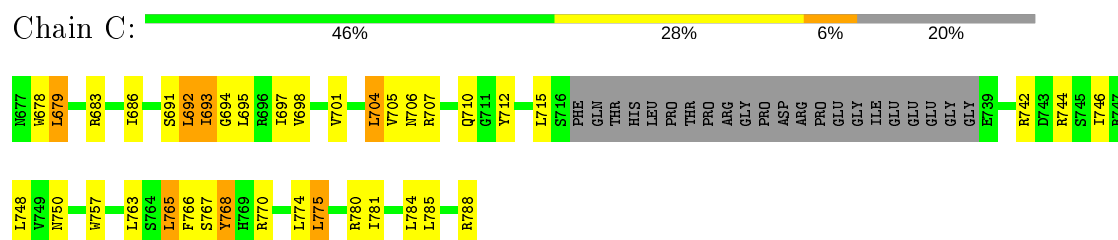
- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41

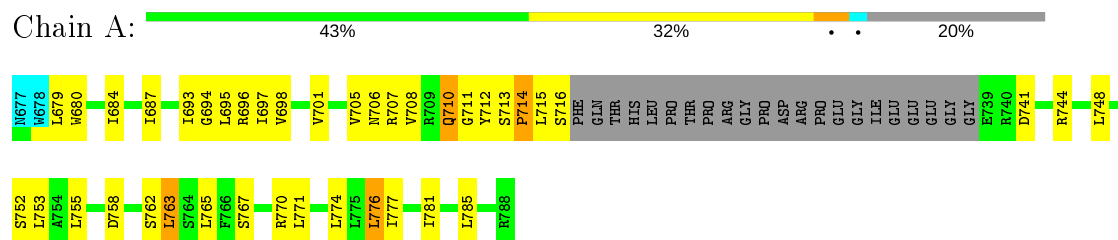


- Molecule 1: Envelope glycoprotein GP41



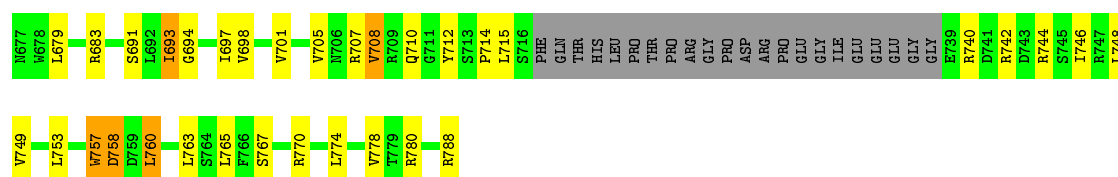
4.2.5 Score per residue for model 5

- Molecule 1: Envelope glycoprotein GP41

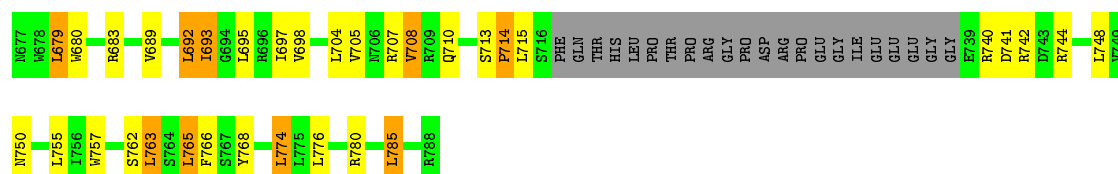


- Molecule 1: Envelope glycoprotein GP41



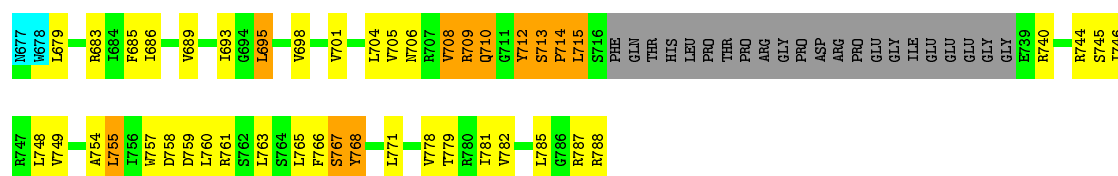


- Molecule 1: Envelope glycoprotein GP41

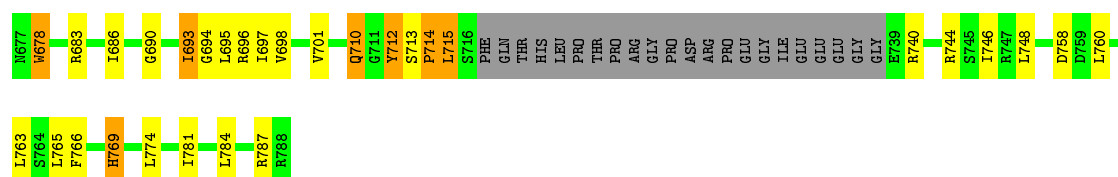


4.2.6 Score per residue for model 6

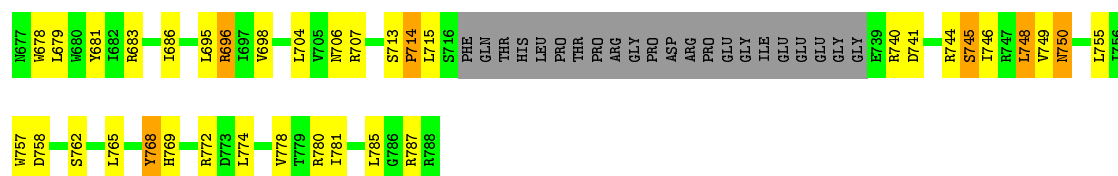
- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41

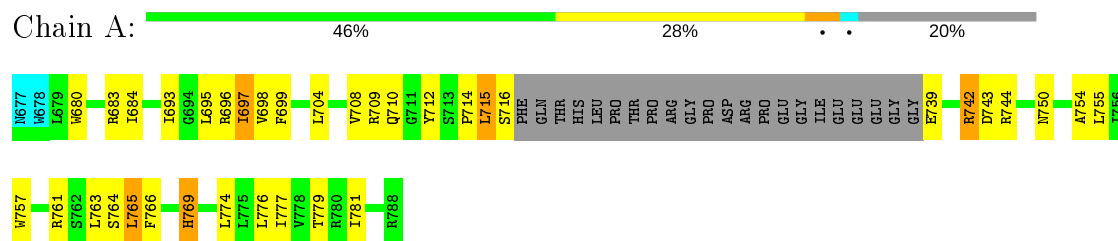


- Molecule 1: Envelope glycoprotein GP41

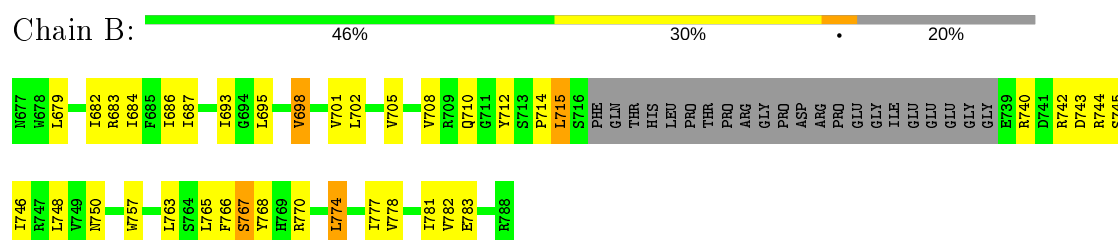


4.2.7 Score per residue for model 7

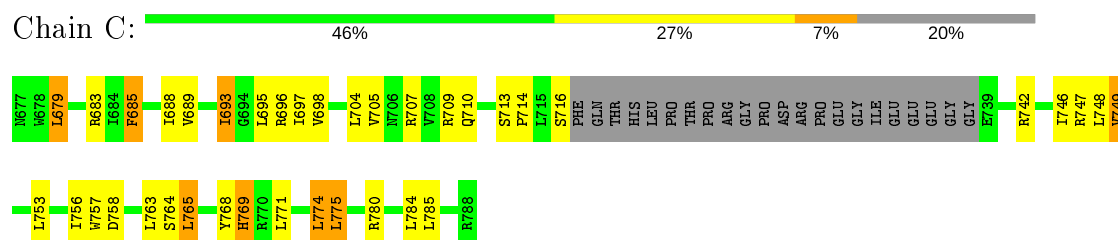
- Molecule 1: Envelope glycoprotein GP41



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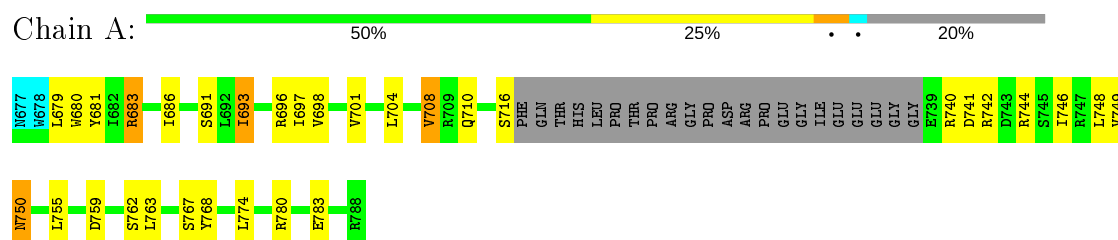


- Molecule 1: Envelope glycoprotein GP41



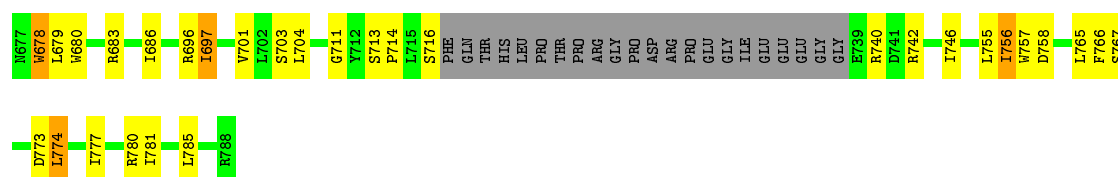
4.2.8 Score per residue for model 8

- Molecule 1: Envelope glycoprotein GP41

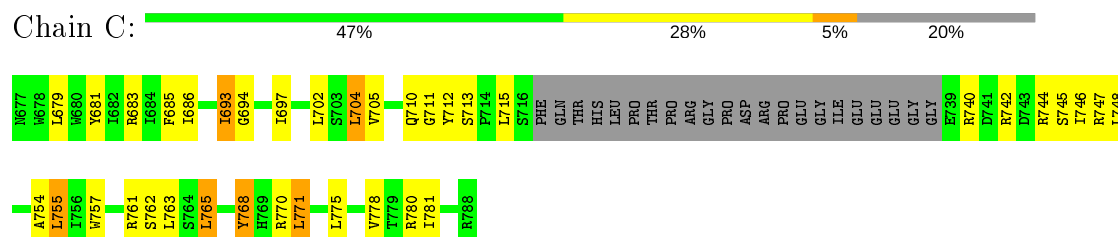


- Molecule 1: Envelope glycoprotein GP41



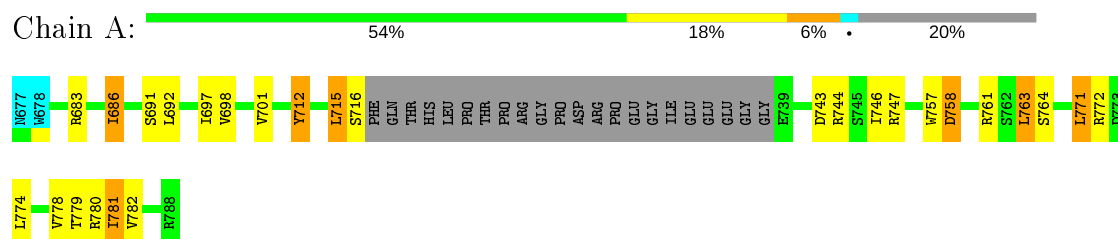


- Molecule 1: Envelope glycoprotein GP41

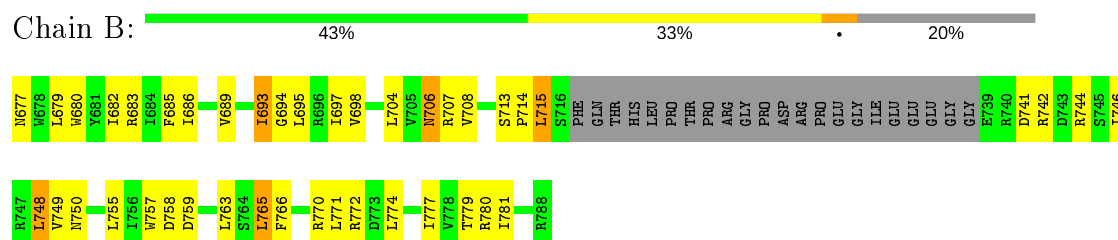


4.2.9 Score per residue for model 9

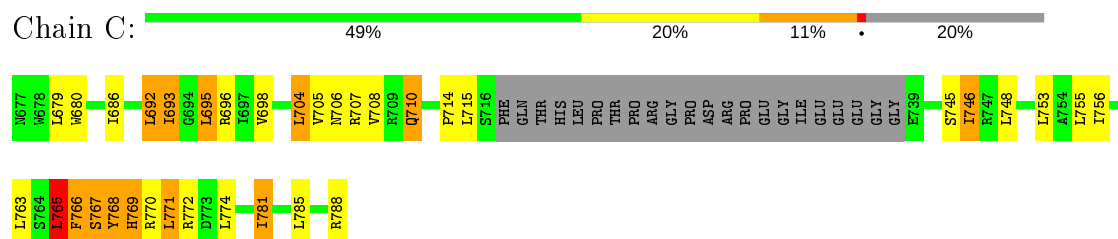
- Molecule 1: Envelope glycoprotein GP41



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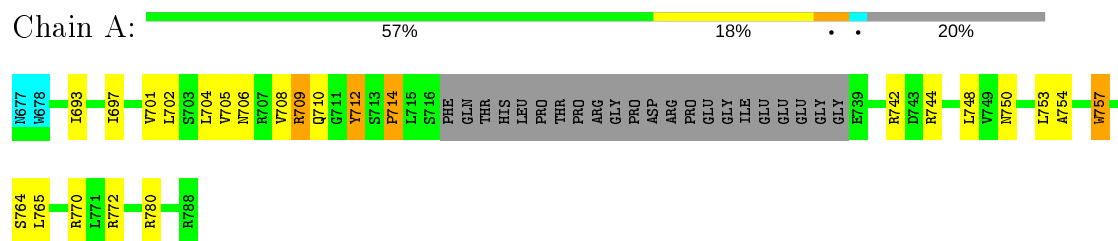


- Molecule 1: Envelope glycoprotein GP41

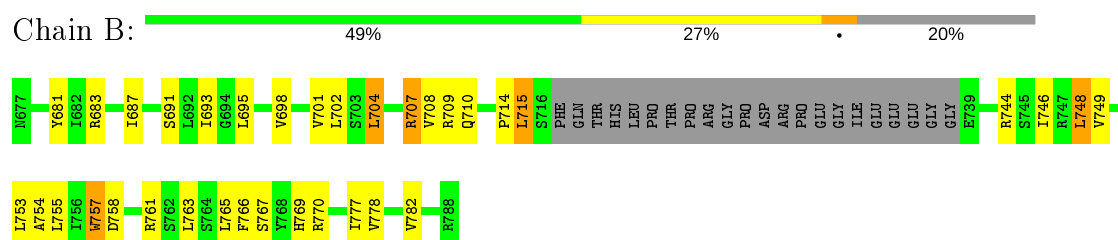


4.2.10 Score per residue for model 10

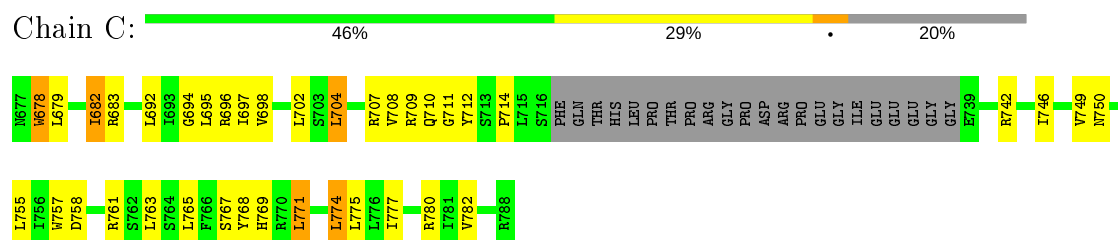
- Molecule 1: Envelope glycoprotein GP41



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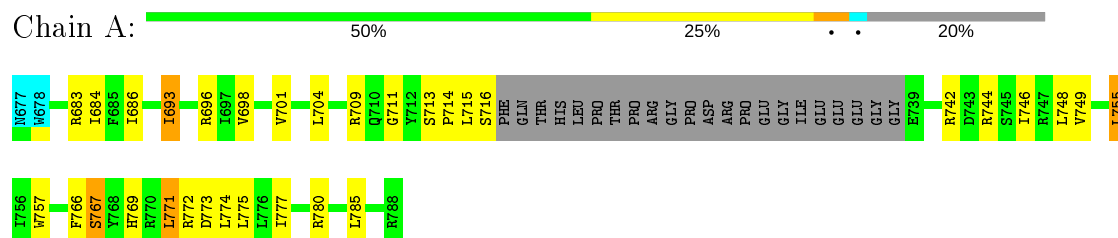


- Molecule 1: Envelope glycoprotein GP41



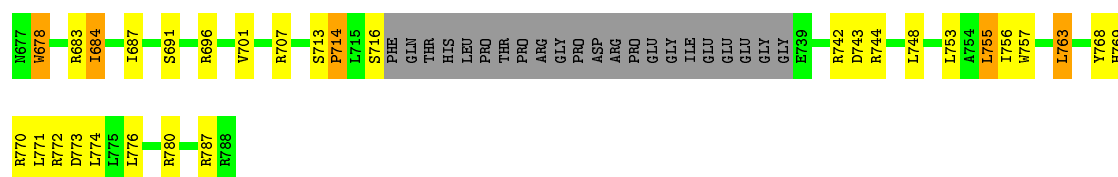
4.2.11 Score per residue for model 11

- Molecule 1: Envelope glycoprotein GP41

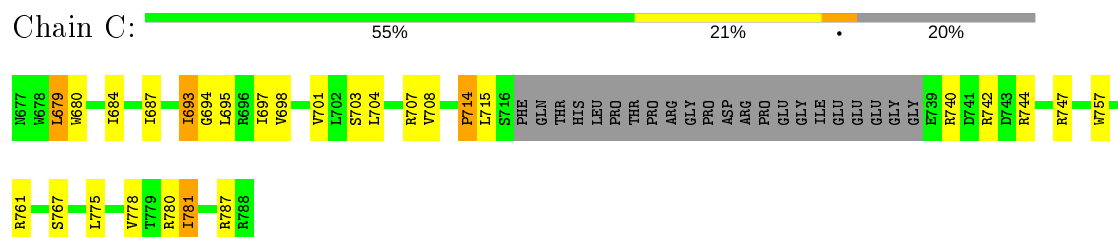


- Molecule 1: Envelope glycoprotein GP41



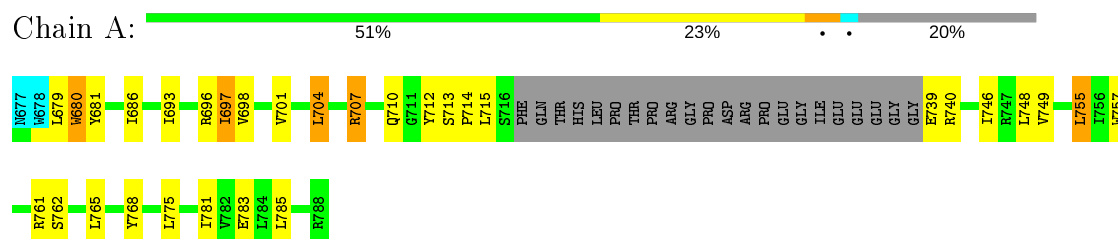


- Molecule 1: Envelope glycoprotein GP41

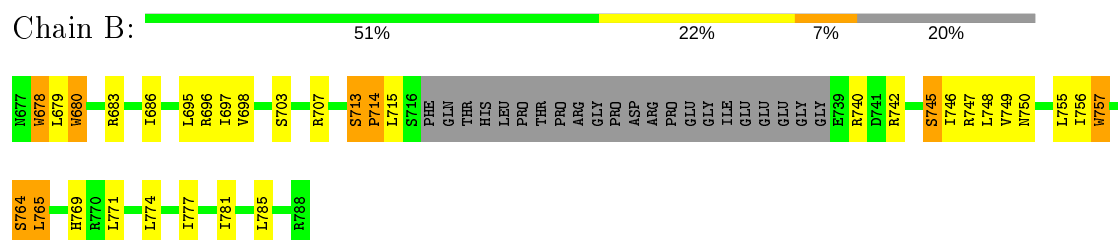


4.2.12 Score per residue for model 12

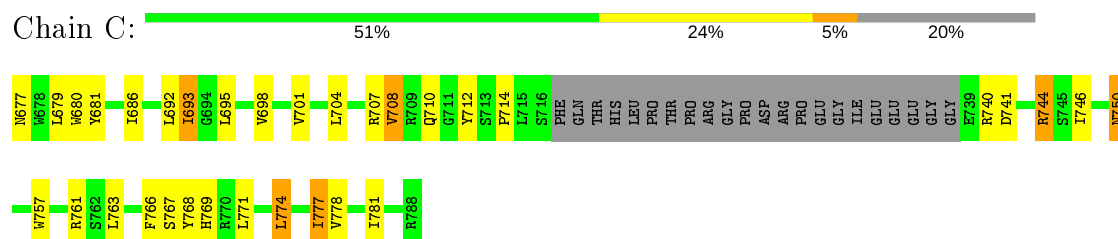
- Molecule 1: Envelope glycoprotein GP41



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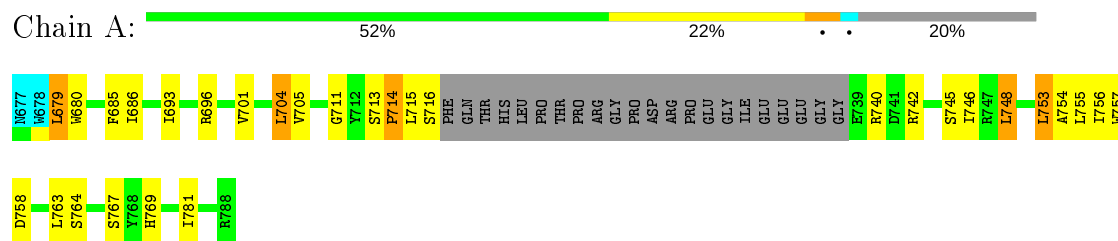


- Molecule 1: Envelope glycoprotein GP41

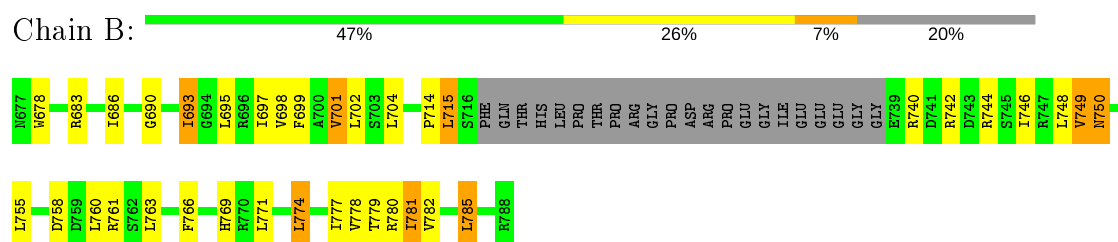


4.2.13 Score per residue for model 13 (medoid)

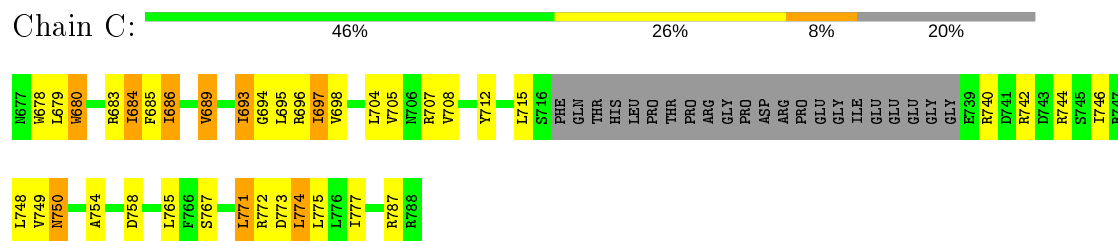
- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41

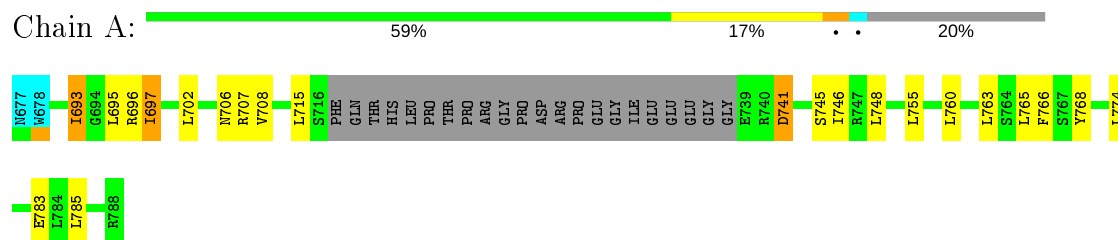


- Molecule 1: Envelope glycoprotein GP41



4.2.14 Score per residue for model 14

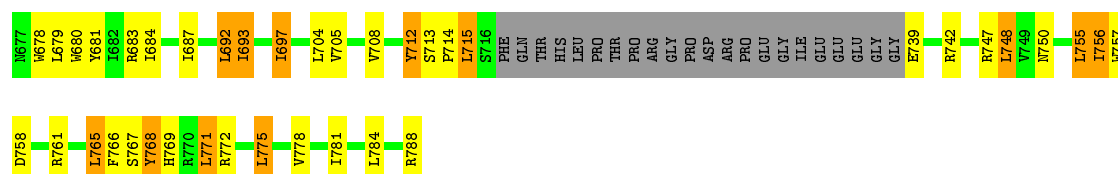
- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41

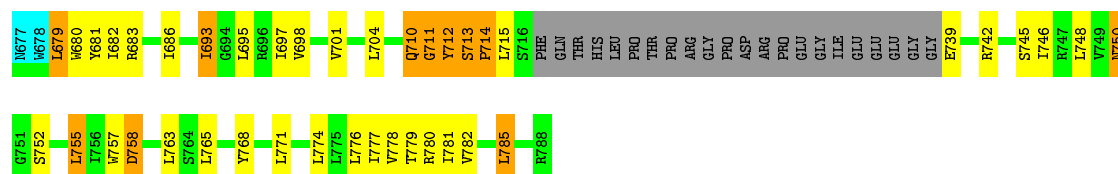


- Molecule 1: Envelope glycoprotein GP41

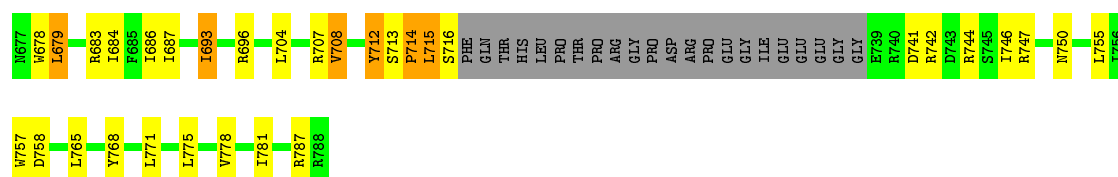


4.2.15 Score per residue for model 15

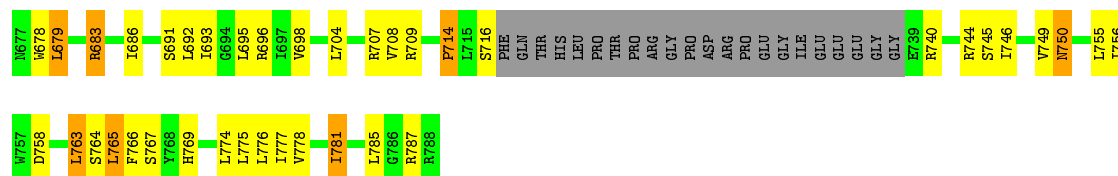
- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41



- Molecule 1: Envelope glycoprotein GP41



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 150 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	460
Number of shifts mapped to atoms	460
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	10%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	731	791	789	19±5
1	B	753	809	804	19±6
1	C	753	809	804	20±5
All	All	33555	36135	35955	693

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:781:ILE:HG23	1:B:746:ILE:HG23	1.06	1.23	12	2
1:A:754:ALA:HB2	1:B:715:LEU:HD22	1.02	1.21	4	1
1:A:746:ILE:HG23	1:C:781:ILE:HD11	0.84	1.49	15	1
1:B:692:LEU:HD13	1:B:693:ILE:N	0.82	1.90	1	1
1:B:746:ILE:O	1:B:749:VAL:HG22	0.81	1.76	3	2
1:B:686:ILE:HG21	1:C:686:ILE:HG23	0.80	1.51	9	1
1:C:748:LEU:HD13	1:C:749:VAL:N	0.75	1.97	6	1
1:B:749:VAL:HG23	1:B:750:ASN:ND2	0.75	1.97	3	1
1:C:698:VAL:O	1:C:701:VAL:HG22	0.74	1.83	12	3
1:A:775:LEU:O	1:A:778:VAL:HG22	0.74	1.83	1	1
1:B:774:LEU:O	1:B:778:VAL:HG23	0.73	1.84	5	2
1:A:746:ILE:HG23	1:C:781:ILE:CD1	0.72	2.14	15	1
1:A:686:ILE:CD1	1:C:686:ILE:HG21	0.72	2.14	6	1
1:A:693:ILE:HD13	1:A:693:ILE:O	0.72	1.83	11	1
1:A:785:LEU:HD22	1:B:746:ILE:HG22	0.71	1.62	12	1
1:A:777:ILE:O	1:A:781:ILE:HD12	0.71	1.85	4	2
1:C:771:LEU:HD13	1:C:772:ARG:N	0.71	2.01	14	3
1:C:775:LEU:O	1:C:778:VAL:HG22	0.70	1.85	15	5
1:A:758:ASP:OD2	1:B:715:LEU:HD12	0.70	1.86	6	1
1:B:779:THR:O	1:B:782:VAL:HG22	0.70	1.86	13	1
1:C:684:ILE:O	1:C:684:ILE:HD13	0.70	1.87	13	1
1:A:710:GLN:OE1	1:C:704:LEU:HD21	0.69	1.87	8	1
1:A:748:LEU:HD11	1:B:714:PRO:CG	0.69	2.18	6	1
1:A:781:ILE:CG2	1:B:746:ILE:HG23	0.68	2.12	12	1
1:A:785:LEU:HD22	1:B:750:ASN:ND2	0.68	2.04	15	1
1:B:698:VAL:O	1:B:701:VAL:HG22	0.68	1.88	6	5
1:C:693:ILE:O	1:C:693:ILE:HD13	0.67	1.89	14	6
1:C:763:LEU:HD22	1:C:764:SER:N	0.67	2.03	15	1
1:A:698:VAL:O	1:A:701:VAL:HG22	0.67	1.89	5	11
1:B:693:ILE:HD11	1:C:696:ARG:NE	0.67	2.04	13	1
1:A:686:ILE:HD12	1:C:686:ILE:HG21	0.66	1.67	6	2
1:A:746:ILE:HD13	1:C:781:ILE:HD12	0.65	1.66	8	1
1:B:778:VAL:O	1:B:781:ILE:HG22	0.65	1.92	13	1
1:B:748:LEU:HD13	1:B:748:LEU:O	0.65	1.92	3	2
1:B:755:LEU:HD13	1:B:756:ILE:N	0.65	2.06	11	1
1:A:771:LEU:O	1:A:771:LEU:HD13	0.65	1.90	2	2
1:C:778:VAL:O	1:C:781:ILE:HG22	0.65	1.92	12	2
1:A:774:LEU:HD13	1:A:774:LEU:H	0.65	1.51	2	1
1:A:755:LEU:O	1:A:755:LEU:HD22	0.65	1.91	3	1
1:B:684:ILE:O	1:B:687:ILE:HG22	0.65	1.92	15	2
1:A:693:ILE:CG2	1:B:693:ILE:HG22	0.64	2.22	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:699:PHE:CG	1:C:697:ILE:HD11	0.64	2.28	7	1
1:B:694:GLY:O	1:B:697:ILE:HG22	0.64	1.93	5	7
1:A:755:LEU:HD22	1:A:755:LEU:O	0.64	1.92	15	4
1:B:686:ILE:HG21	1:C:686:ILE:HD12	0.64	1.69	12	1
1:C:774:LEU:HD13	1:C:777:ILE:HD12	0.64	1.70	12	1
1:A:704:LEU:HD11	1:B:707:ARG:NE	0.63	2.08	10	1
1:A:771:LEU:HD13	1:A:771:LEU:O	0.63	1.93	6	1
1:A:785:LEU:HD23	1:B:750:ASN:ND2	0.63	2.08	12	1
1:B:710:GLN:O	1:B:715:LEU:HD12	0.63	1.94	1	1
1:C:679:LEU:HD13	1:C:679:LEU:O	0.63	1.94	11	5
1:C:697:ILE:HD13	1:C:697:ILE:O	0.63	1.93	13	1
1:B:686:ILE:HG23	1:C:686:ILE:CD1	0.63	2.24	13	2
1:A:679:LEU:HD22	1:A:680:TRP:N	0.63	2.08	13	1
1:B:705:VAL:HG22	1:B:748:LEU:HD22	0.63	1.71	14	1
1:A:779:THR:O	1:A:782:VAL:HG22	0.63	1.94	9	3
1:A:693:ILE:HG21	1:B:693:ILE:HG22	0.62	1.71	2	3
1:A:695:LEU:C	1:A:695:LEU:HD22	0.62	2.15	6	1
1:B:774:LEU:HD22	1:B:777:ILE:HD11	0.62	1.69	13	3
1:C:705:VAL:HG22	1:C:748:LEU:HD11	0.62	1.71	13	2
1:C:708:VAL:HG12	1:C:748:LEU:HD11	0.62	1.70	5	1
1:C:679:LEU:O	1:C:679:LEU:HD13	0.62	1.95	10	2
1:C:693:ILE:O	1:C:693:ILE:HD12	0.62	1.94	12	1
1:A:695:LEU:HD22	1:A:695:LEU:O	0.61	1.94	6	1
1:C:755:LEU:HD22	1:C:755:LEU:C	0.61	2.15	14	1
1:A:694:GLY:O	1:A:697:ILE:HG22	0.61	1.94	5	2
1:C:775:LEU:O	1:C:775:LEU:HD13	0.61	1.96	10	2
1:B:763:LEU:O	1:B:774:LEU:HD13	0.61	1.95	6	3
1:A:697:ILE:O	1:A:697:ILE:HD13	0.61	1.95	12	2
1:B:697:ILE:O	1:B:697:ILE:HD13	0.61	1.95	8	1
1:C:697:ILE:O	1:C:697:ILE:HD13	0.61	1.96	14	1
1:B:679:LEU:O	1:B:679:LEU:HD13	0.61	1.96	1	2
1:C:777:ILE:HD12	1:C:778:VAL:N	0.61	2.11	15	1
1:A:771:LEU:HD23	1:A:771:LEU:O	0.61	1.95	15	1
1:A:697:ILE:HD13	1:A:697:ILE:O	0.61	1.96	14	1
1:C:710:GLN:CB	1:C:715:LEU:HD23	0.61	2.25	2	1
1:C:695:LEU:O	1:C:698:VAL:HG12	0.60	1.96	9	9
1:B:781:ILE:HD12	1:C:746:ILE:HG21	0.60	1.72	3	3
1:C:768:TYR:O	1:C:771:LEU:HD12	0.60	1.95	14	1
1:B:697:ILE:HD13	1:B:697:ILE:O	0.60	1.96	4	2
1:A:754:ALA:CB	1:B:715:LEU:HD22	0.60	2.14	4	1
1:A:679:LEU:HD13	1:A:680:TRP:H	0.60	1.56	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:696:ARG:HG3	1:C:693:ILE:HD11	0.60	1.74	1	4
1:C:748:LEU:O	1:C:748:LEU:HD13	0.60	1.96	1	1
1:A:686:ILE:CG2	1:B:686:ILE:HD12	0.60	2.26	2	1
1:A:705:VAL:HG22	1:A:748:LEU:HD12	0.60	1.74	4	1
1:A:755:LEU:HD23	1:B:710:GLN:HE21	0.60	1.54	3	1
1:B:771:LEU:HD23	1:B:771:LEU:O	0.60	1.97	3	2
1:A:679:LEU:HD13	1:A:680:TRP:N	0.60	2.12	15	1
1:B:710:GLN:HG3	1:B:715:LEU:HD13	0.59	1.74	6	1
1:A:679:LEU:HD12	1:A:680:TRP:N	0.59	2.13	12	2
1:C:695:LEU:HD23	1:C:695:LEU:O	0.59	1.97	4	4
1:A:695:LEU:O	1:A:698:VAL:HG12	0.59	1.98	6	4
1:A:746:ILE:HG23	1:C:781:ILE:CG1	0.59	2.28	15	1
1:B:758:ASP:CG	1:C:715:LEU:HD21	0.59	2.18	1	2
1:A:778:VAL:O	1:A:781:ILE:HG22	0.59	1.98	9	1
1:C:705:VAL:HG22	1:C:748:LEU:CD1	0.59	2.27	13	1
1:C:746:ILE:O	1:C:749:VAL:HG22	0.58	1.98	15	4
1:A:748:LEU:HD11	1:B:714:PRO:HG3	0.58	1.73	6	1
1:A:776:LEU:O	1:A:779:THR:HG22	0.58	1.97	7	2
1:C:771:LEU:HD22	1:C:772:ARG:N	0.58	2.13	13	1
1:B:686:ILE:CG2	1:C:686:ILE:HD12	0.58	2.28	12	3
1:A:696:ARG:HE	1:C:693:ILE:HD11	0.58	1.57	12	3
1:B:781:ILE:HG21	1:C:746:ILE:CG2	0.58	2.29	9	3
1:B:698:VAL:O	1:B:701:VAL:HG12	0.58	1.98	13	1
1:A:704:LEU:CD2	1:A:755:LEU:HD23	0.58	2.29	6	1
1:B:755:LEU:O	1:B:755:LEU:HD22	0.58	1.99	11	1
1:B:755:LEU:HA	1:C:715:LEU:HD23	0.58	1.74	1	1
1:C:715:LEU:O	1:C:715:LEU:HD13	0.58	1.99	2	1
1:A:755:LEU:HD23	1:B:710:GLN:NE2	0.58	2.14	3	1
1:C:695:LEU:C	1:C:695:LEU:HD22	0.58	2.18	9	1
1:A:776:LEU:O	1:A:776:LEU:HD22	0.57	1.99	5	1
1:B:774:LEU:CD2	1:B:777:ILE:HD11	0.57	2.29	12	2
1:C:756:ILE:HD12	1:C:757:TRP:N	0.57	2.14	7	1
1:C:694:GLY:O	1:C:697:ILE:HG22	0.57	1.99	8	6
1:A:754:ALA:O	1:B:715:LEU:HD11	0.57	1.99	6	1
1:A:697:ILE:HD11	1:B:696:ARG:NH2	0.57	2.15	8	1
1:C:708:VAL:CG1	1:C:748:LEU:HD11	0.57	2.29	5	1
1:C:775:LEU:HD13	1:C:775:LEU:O	0.57	1.99	1	2
1:A:745:SER:HA	1:A:748:LEU:HD13	0.57	1.76	6	1
1:A:704:LEU:HD22	1:A:755:LEU:HD23	0.57	1.77	6	1
1:A:713:SER:CB	1:C:708:VAL:HG23	0.56	2.30	12	2
1:A:776:LEU:HD13	1:A:777:ILE:N	0.56	2.15	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:777:ILE:O	1:A:781:ILE:HD13	0.56	1.99	15	1
1:B:707:ARG:NH1	1:B:708:VAL:HG23	0.56	2.14	5	1
1:A:774:LEU:HD21	1:B:742:ARG:NH2	0.56	2.15	11	1
1:B:776:LEU:O	1:B:779:THR:HG22	0.56	1.99	1	1
1:C:756:ILE:HD13	1:C:756:ILE:O	0.56	2.01	1	1
1:A:754:ALA:HB3	1:B:715:LEU:HD13	0.56	1.77	2	1
1:B:715:LEU:HD23	1:B:715:LEU:H	0.56	1.60	5	1
1:B:785:LEU:HD21	1:C:750:ASN:ND2	0.56	2.15	12	2
1:A:771:LEU:O	1:A:771:LEU:HD23	0.56	2.00	1	1
1:B:758:ASP:CB	1:C:715:LEU:HD21	0.56	2.31	1	1
1:B:758:ASP:OD2	1:C:715:LEU:HD22	0.56	2.00	6	1
1:B:774:LEU:O	1:B:774:LEU:HD13	0.56	2.00	11	1
1:A:746:ILE:CG2	1:C:781:ILE:HD11	0.56	2.28	15	1
1:C:693:ILE:HD12	1:C:693:ILE:O	0.56	2.01	8	1
1:B:774:LEU:HD21	1:C:742:ARG:NE	0.55	2.16	11	1
1:A:753:LEU:HD21	1:A:757:TRP:CZ3	0.55	2.36	13	1
1:C:765:LEU:HD13	1:C:765:LEU:O	0.55	2.02	9	1
1:A:774:LEU:HD22	1:A:775:LEU:N	0.55	2.16	2	1
1:C:768:TYR:CD1	1:C:771:LEU:HD21	0.55	2.37	8	1
1:A:686:ILE:HG21	1:B:686:ILE:HG13	0.55	1.76	13	1
1:B:781:ILE:HD12	1:C:746:ILE:HG23	0.55	1.78	8	1
1:B:686:ILE:HG22	1:C:686:ILE:HD12	0.55	1.79	4	1
1:A:748:LEU:HD23	1:A:748:LEU:O	0.55	2.01	5	1
1:A:705:VAL:HG13	1:A:748:LEU:HD13	0.55	1.78	10	1
1:A:758:ASP:OD1	1:B:715:LEU:HD23	0.55	2.01	13	1
1:C:710:GLN:O	1:C:715:LEU:HD22	0.55	2.02	1	1
1:A:684:ILE:HD13	1:A:684:ILE:O	0.55	2.02	3	2
1:A:746:ILE:CG2	1:C:781:ILE:HG21	0.54	2.32	1	3
1:C:746:ILE:O	1:C:749:VAL:HG23	0.54	2.02	13	2
1:A:711:GLY:HA3	1:A:715:LEU:HD13	0.54	1.79	15	2
1:C:748:LEU:HD13	1:C:748:LEU:O	0.54	2.01	14	1
1:C:755:LEU:HD22	1:C:755:LEU:O	0.54	2.03	8	1
1:B:686:ILE:HG23	1:C:686:ILE:HD11	0.54	1.79	13	1
1:A:693:ILE:O	1:A:693:ILE:HD12	0.54	2.03	15	2
1:A:746:ILE:O	1:A:749:VAL:HG22	0.54	2.03	8	2
1:A:693:ILE:HD11	1:B:692:LEU:HD23	0.54	1.79	14	2
1:C:768:TYR:O	1:C:770:ARG:N	0.54	2.41	2	1
1:B:693:ILE:O	1:B:693:ILE:HD12	0.54	2.03	9	3
1:A:754:ALA:HB1	1:B:715:LEU:CD1	0.54	2.32	7	1
1:C:710:GLN:O	1:C:715:LEU:HD13	0.54	2.03	1	1
1:A:781:ILE:HD13	1:B:746:ILE:HG21	0.53	1.81	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:715:LEU:HD22	1:B:715:LEU:O	0.53	2.03	13	1
1:C:693:ILE:HD13	1:C:693:ILE:O	0.53	2.03	4	2
1:B:757:TRP:CZ3	1:B:760:LEU:HD13	0.53	2.38	5	1
1:A:716:SER:HA	1:C:754:ALA:HB2	0.53	1.80	8	2
1:B:781:ILE:HG21	1:C:747:ARG:HH12	0.53	1.63	14	1
1:A:686:ILE:HG23	1:C:686:ILE:HG21	0.53	1.81	8	2
1:B:763:LEU:HA	1:B:774:LEU:HD22	0.53	1.79	4	2
1:B:695:LEU:O	1:B:695:LEU:HD23	0.53	2.04	12	3
1:A:771:LEU:HD22	1:A:771:LEU:C	0.53	2.24	11	1
1:B:708:VAL:HG11	1:C:714:PRO:HD3	0.53	1.81	7	1
1:B:755:LEU:HD21	1:C:710:GLN:NE2	0.52	2.18	1	2
1:C:710:GLN:HB3	1:C:715:LEU:HD23	0.52	1.80	2	1
1:A:696:ARG:NE	1:C:693:ILE:HD11	0.52	2.19	5	2
1:A:679:LEU:HD22	1:A:679:LEU:C	0.52	2.25	15	2
1:B:708:VAL:HG12	1:B:748:LEU:HD11	0.52	1.81	4	1
1:B:748:LEU:O	1:B:748:LEU:HD13	0.52	2.05	10	1
1:B:715:LEU:HD23	1:B:716:SER:N	0.52	2.19	4	1
1:A:710:GLN:O	1:A:715:LEU:HD21	0.52	2.04	7	1
1:C:774:LEU:HD13	1:C:777:ILE:CD1	0.52	2.35	12	1
1:A:693:ILE:HD11	1:B:696:ARG:HG3	0.52	1.80	11	1
1:A:685:PHE:O	1:A:689:VAL:HG23	0.52	2.05	6	1
1:A:708:VAL:HG21	1:B:714:PRO:CD	0.52	2.35	14	4
1:A:781:ILE:HD12	1:B:746:ILE:CG2	0.52	2.35	6	1
1:B:758:ASP:CG	1:C:710:GLN:HB2	0.52	2.25	9	1
1:A:713:SER:HB3	1:C:708:VAL:HG23	0.52	1.82	1	1
1:B:708:VAL:HG21	1:C:714:PRO:CD	0.51	2.35	15	2
1:B:778:VAL:O	1:B:782:VAL:HG23	0.51	2.05	14	4
1:C:692:LEU:HD12	1:C:693:ILE:N	0.51	2.20	5	2
1:C:771:LEU:C	1:C:771:LEU:HD22	0.51	2.25	13	3
1:C:771:LEU:HD22	1:C:771:LEU:C	0.51	2.25	3	1
1:B:758:ASP:HB2	1:C:715:LEU:HD21	0.51	1.82	1	1
1:C:679:LEU:O	1:C:679:LEU:HD23	0.51	2.04	14	1
1:B:774:LEU:HD13	1:B:777:ILE:HD11	0.51	1.83	8	1
1:A:763:LEU:N	1:A:763:LEU:HD13	0.51	2.20	9	1
1:B:748:LEU:HD11	1:C:714:PRO:HG3	0.51	1.83	11	1
1:B:693:ILE:HD11	1:C:692:LEU:HD23	0.51	1.82	10	3
1:C:763:LEU:O	1:C:774:LEU:HD13	0.51	2.05	5	1
1:B:774:LEU:HD13	1:B:774:LEU:O	0.51	2.06	7	1
1:B:748:LEU:HD11	1:C:714:PRO:CG	0.51	2.35	11	1
1:A:771:LEU:HD22	1:A:772:ARG:N	0.50	2.21	11	1
1:A:713:SER:OG	1:C:708:VAL:HG23	0.50	2.06	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:705:VAL:HG13	1:C:748:LEU:HD21	0.50	1.82	7	1
1:A:713:SER:HB2	1:C:708:VAL:HG23	0.50	1.82	12	1
1:A:693:ILE:HD11	1:B:696:ARG:CG	0.50	2.36	11	1
1:A:711:GLY:HA3	1:A:715:LEU:HD21	0.50	1.84	5	1
1:C:692:LEU:HD12	1:C:693:ILE:H	0.50	1.66	5	2
1:B:693:ILE:HD11	1:C:696:ARG:HG3	0.50	1.83	15	2
1:B:746:ILE:O	1:B:749:VAL:HG12	0.50	2.06	5	2
1:A:754:ALA:HA	1:B:715:LEU:HD23	0.50	1.83	10	1
1:B:774:LEU:C	1:B:774:LEU:HD13	0.50	2.27	14	3
1:A:781:ILE:HD12	1:B:746:ILE:HG21	0.50	1.83	1	2
1:B:695:LEU:O	1:B:698:VAL:HG12	0.50	2.07	10	5
1:C:771:LEU:HD13	1:C:772:ARG:H	0.50	1.67	14	3
1:B:745:SER:O	1:B:748:LEU:HD23	0.49	2.06	7	1
1:C:704:LEU:HD13	1:C:704:LEU:O	0.49	2.07	9	2
1:B:748:LEU:HD13	1:B:748:LEU:C	0.49	2.27	3	1
1:B:704:LEU:HD11	1:B:707:ARG:NH1	0.49	2.23	9	1
1:A:746:ILE:HD13	1:C:781:ILE:CD1	0.49	2.36	8	1
1:A:704:LEU:HD13	1:A:704:LEU:O	0.49	2.07	4	1
1:A:705:VAL:HG22	1:A:748:LEU:HD22	0.49	1.84	5	1
1:C:705:VAL:HG13	1:C:748:LEU:HD13	0.49	1.85	8	2
1:C:713:SER:O	1:C:715:LEU:HD22	0.49	2.08	8	1
1:A:774:LEU:O	1:A:778:VAL:HG23	0.49	2.08	9	2
1:A:774:LEU:HD22	1:A:777:ILE:HD11	0.49	1.84	11	1
1:A:763:LEU:O	1:A:774:LEU:HD22	0.49	2.07	1	1
1:A:742:ARG:CZ	1:C:774:LEU:HD21	0.49	2.37	7	1
1:A:710:GLN:NE2	1:C:755:LEU:HD21	0.49	2.23	8	1
1:A:686:ILE:CG2	1:B:686:ILE:HD11	0.49	2.37	9	1
1:B:715:LEU:O	1:B:716:SER:C	0.49	2.50	14	1
1:A:710:GLN:CD	1:C:704:LEU:HD21	0.49	2.28	8	1
1:C:774:LEU:HD22	1:C:777:ILE:HD11	0.48	1.84	10	2
1:B:755:LEU:HD23	1:B:755:LEU:O	0.48	2.08	13	1
1:A:785:LEU:HD21	1:B:746:ILE:HG22	0.48	1.85	15	1
1:A:750:ASN:OD1	1:C:785:LEU:HD22	0.48	2.08	2	1
1:A:746:ILE:O	1:A:749:VAL:HG23	0.48	2.08	6	3
1:B:715:LEU:C	1:B:715:LEU:HD22	0.48	2.28	13	1
1:A:705:VAL:HG22	1:A:748:LEU:HD13	0.48	1.83	1	1
1:B:775:LEU:C	1:B:775:LEU:HD13	0.48	2.29	3	1
1:A:686:ILE:CG1	1:C:686:ILE:HG21	0.48	2.39	9	1
1:C:704:LEU:O	1:C:704:LEU:HD13	0.48	2.08	4	1
1:A:754:ALA:HB1	1:B:715:LEU:HD21	0.48	1.85	13	1
1:C:763:LEU:O	1:C:774:LEU:HD22	0.48	2.09	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:708:VAL:HG21	1:B:714:PRO:HD3	0.48	1.84	6	3
1:C:697:ILE:C	1:C:697:ILE:HD13	0.48	2.29	3	1
1:A:755:LEU:HD22	1:B:710:GLN:OE1	0.48	2.09	4	1
1:B:684:ILE:HD13	1:B:684:ILE:O	0.48	2.09	4	1
1:C:679:LEU:HD13	1:C:679:LEU:C	0.48	2.28	9	2
1:C:707:ARG:NH2	1:C:708:VAL:HG23	0.48	2.24	13	1
1:B:715:LEU:HD13	1:B:715:LEU:H	0.47	1.68	1	1
1:B:781:ILE:HG21	1:C:746:ILE:HG23	0.47	1.86	6	2
1:A:686:ILE:HD12	1:C:686:ILE:CG2	0.47	2.39	12	1
1:A:758:ASP:HB3	1:B:715:LEU:HD13	0.47	1.86	15	1
1:B:781:ILE:CD1	1:C:746:ILE:HG21	0.47	2.37	4	1
1:B:771:LEU:O	1:B:771:LEU:HD23	0.47	2.09	13	1
1:A:776:LEU:HD13	1:A:776:LEU:C	0.47	2.29	2	2
1:A:715:LEU:O	1:A:716:SER:C	0.47	2.51	5	4
1:B:774:LEU:HD21	1:C:742:ARG:HE	0.47	1.68	11	1
1:B:781:ILE:HD12	1:C:746:ILE:CG2	0.47	2.39	3	1
1:C:765:LEU:HD13	1:C:765:LEU:C	0.47	2.29	13	1
1:A:715:LEU:HD21	1:C:758:ASP:OD2	0.47	2.09	14	1
1:A:693:ILE:HG22	1:C:693:ILE:HG13	0.47	1.84	13	3
1:B:695:LEU:O	1:B:698:VAL:HG22	0.47	2.10	12	1
1:A:754:ALA:CB	1:B:715:LEU:HD21	0.47	2.39	13	1
1:A:695:LEU:C	1:A:695:LEU:HD23	0.47	2.30	5	1
1:B:763:LEU:HD13	1:B:763:LEU:H	0.47	1.69	11	1
1:B:707:ARG:CZ	1:C:707:ARG:CZ	0.47	2.93	2	1
1:C:774:LEU:O	1:C:774:LEU:HD13	0.46	2.09	10	2
1:C:785:LEU:O	1:C:785:LEU:HD13	0.46	2.11	5	1
1:B:781:ILE:HD13	1:C:746:ILE:HG21	0.46	1.87	13	1
1:A:746:ILE:HG21	1:C:781:ILE:HG21	0.46	1.86	1	1
1:A:703:SER:O	1:A:707:ARG:HG3	0.46	2.10	2	1
1:B:754:ALA:HB1	1:C:710:GLN:OE1	0.46	2.10	10	1
1:C:745:SER:O	1:C:748:LEU:HD12	0.46	2.11	6	1
1:B:781:ILE:HG13	1:C:746:ILE:HG21	0.46	1.87	6	1
1:A:715:LEU:N	1:A:715:LEU:HD22	0.46	2.25	7	1
1:A:754:ALA:CB	1:B:715:LEU:HD23	0.46	2.40	10	1
1:C:764:SER:O	1:C:765:LEU:CB	0.46	2.64	7	1
1:A:774:LEU:CD2	1:A:777:ILE:HD11	0.46	2.40	11	1
1:B:693:ILE:HD12	1:B:693:ILE:O	0.46	2.10	13	1
1:A:710:GLN:O	1:A:715:LEU:HD11	0.46	2.11	7	1
1:B:682:ILE:O	1:B:686:ILE:HD13	0.46	2.10	7	1
1:B:713:SER:O	1:B:714:PRO:C	0.46	2.53	11	4
1:A:693:ILE:HG22	1:C:693:ILE:CG1	0.46	2.40	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:693:ILE:HD11	1:C:696:ARG:HG2	0.46	1.87	6	1
1:A:686:ILE:HG21	1:B:686:ILE:HG12	0.46	1.88	8	1
1:C:705:VAL:HG12	1:C:748:LEU:HD23	0.46	1.88	9	1
1:B:781:ILE:HG13	1:C:746:ILE:HD12	0.46	1.87	12	1
1:A:781:ILE:CD1	1:B:746:ILE:HG21	0.46	2.41	7	2
1:B:708:VAL:CG1	1:B:748:LEU:HD11	0.46	2.41	4	1
1:C:774:LEU:C	1:C:774:LEU:HD13	0.46	2.30	4	1
1:B:690:GLY:O	1:B:693:ILE:HG23	0.46	2.10	13	2
1:B:781:ILE:HG21	1:C:746:ILE:HG21	0.46	1.87	9	1
1:C:755:LEU:HD13	1:C:756:ILE:N	0.46	2.26	14	1
1:C:776:LEU:C	1:C:776:LEU:HD13	0.45	2.32	2	1
1:A:705:VAL:HG22	1:A:748:LEU:CD1	0.45	2.41	4	1
1:A:746:ILE:CG2	1:C:781:ILE:HD13	0.45	2.40	9	1
1:B:695:LEU:C	1:B:695:LEU:HD23	0.45	2.31	12	1
1:A:695:LEU:O	1:A:695:LEU:HD23	0.45	2.11	14	1
1:B:711:GLY:O	1:B:713:SER:N	0.45	2.49	4	1
1:A:704:LEU:HD11	1:B:707:ARG:CZ	0.45	2.42	10	1
1:B:774:LEU:HD13	1:B:774:LEU:C	0.45	2.31	13	1
1:B:705:VAL:CG2	1:B:748:LEU:HD22	0.45	2.40	14	1
1:C:749:VAL:HG23	1:C:750:ASN:N	0.45	2.26	1	3
1:A:712:TYR:CZ	1:B:712:TYR:CE1	0.45	3.04	15	1
1:C:748:LEU:C	1:C:748:LEU:HD22	0.45	2.32	6	1
1:C:692:LEU:O	1:C:695:LEU:HD13	0.45	2.12	9	1
1:B:697:ILE:HD11	1:C:696:ARG:NH2	0.45	2.27	13	1
1:A:713:SER:O	1:A:714:PRO:C	0.45	2.55	5	7
1:A:716:SER:C	1:C:754:ALA:HB2	0.45	2.32	2	1
1:A:781:ILE:HD12	1:B:746:ILE:HG23	0.45	1.87	6	1
1:A:754:ALA:CA	1:B:715:LEU:HD23	0.45	2.42	10	1
1:B:771:LEU:C	1:B:771:LEU:HD13	0.45	2.32	11	1
1:A:755:LEU:HD13	1:A:755:LEU:C	0.45	2.32	13	2
1:B:771:LEU:HD23	1:B:771:LEU:N	0.45	2.27	4	1
1:A:709:ARG:HH22	1:C:755:LEU:HD22	0.45	1.71	10	1
1:B:689:VAL:O	1:B:692:LEU:HD12	0.45	2.12	1	1
1:A:774:LEU:HD13	1:A:774:LEU:C	0.45	2.32	3	1
1:A:710:GLN:HE21	1:C:755:LEU:HD21	0.45	1.71	8	2
1:B:748:LEU:HD23	1:B:748:LEU:O	0.45	2.12	9	1
1:B:679:LEU:HD13	1:B:679:LEU:O	0.45	2.12	15	1
1:C:774:LEU:O	1:C:777:ILE:HG13	0.45	2.12	15	1
1:A:684:ILE:HA	1:A:687:ILE:HD12	0.45	1.89	5	2
1:A:711:GLY:CA	1:A:715:LEU:HD13	0.45	2.42	11	1
1:A:764:SER:O	1:A:770:ARG:HB3	0.44	2.12	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:679:LEU:O	1:A:683:ARG:N	0.44	2.50	8	2
1:A:686:ILE:HD12	1:C:686:ILE:HG22	0.44	1.88	12	1
1:C:684:ILE:HA	1:C:687:ILE:HD12	0.44	1.88	14	1
1:C:704:LEU:C	1:C:704:LEU:HD13	0.44	2.32	14	1
1:A:784:LEU:C	1:A:784:LEU:HD12	0.44	2.33	4	1
1:B:706:ASN:O	1:B:710:GLN:CB	0.44	2.65	4	1
1:C:705:VAL:HG13	1:C:748:LEU:HG	0.44	1.89	14	1
1:A:758:ASP:OD2	1:B:715:LEU:HD13	0.44	2.12	9	1
1:B:755:LEU:C	1:B:755:LEU:HD22	0.44	2.33	11	1
1:B:686:ILE:HG13	1:C:686:ILE:HD12	0.44	1.89	6	1
1:A:785:LEU:HD21	1:B:747:ARG:HA	0.44	1.89	12	1
1:B:686:ILE:O	1:C:686:ILE:HD11	0.44	2.12	13	1
1:A:746:ILE:HD12	1:A:746:ILE:N	0.44	2.27	14	1
1:C:711:GLY:O	1:C:713:SER:N	0.44	2.51	8	1
1:B:695:LEU:HD22	1:B:696:ARG:NH1	0.44	2.28	12	1
1:A:708:VAL:HG21	1:B:714:PRO:HD2	0.44	1.89	14	1
1:C:705:VAL:HG22	1:C:748:LEU:HD21	0.44	1.90	14	1
1:A:776:LEU:HD23	1:A:776:LEU:O	0.44	2.13	3	1
1:C:693:ILE:C	1:C:693:ILE:HD13	0.44	2.32	14	1
1:A:765:LEU:HD13	1:A:765:LEU:C	0.44	2.32	1	1
1:A:704:LEU:HD13	1:A:707:ARG:NH2	0.44	2.27	12	1
1:B:692:LEU:C	1:B:692:LEU:HD13	0.43	2.31	1	1
1:A:763:LEU:O	1:A:774:LEU:HD13	0.43	2.13	5	2
1:B:755:LEU:C	1:B:755:LEU:HD23	0.43	2.34	8	3
1:C:766:PHE:O	1:C:767:SER:O	0.43	2.36	9	1
1:A:714:PRO:HD2	1:C:708:VAL:HG21	0.43	1.90	10	1
1:A:693:ILE:HD11	1:B:696:ARG:HE	0.43	1.73	15	1
1:C:763:LEU:C	1:C:763:LEU:HD22	0.43	2.33	15	1
1:B:710:GLN:O	1:B:715:LEU:HD22	0.43	2.13	5	1
1:C:705:VAL:HG13	1:C:748:LEU:CD1	0.43	2.43	4	1
1:A:705:VAL:HG12	1:A:709:ARG:HG2	0.43	1.89	6	1
1:C:763:LEU:HD13	1:C:763:LEU:H	0.43	1.74	15	1
1:A:781:ILE:HG21	1:B:746:ILE:CG2	0.43	2.43	2	1
1:A:706:ASN:O	1:A:710:GLN:CB	0.43	2.66	6	2
1:B:778:VAL:HG23	1:C:749:VAL:HG21	0.43	1.90	10	1
1:B:746:ILE:O	1:B:749:VAL:HG23	0.43	2.13	10	4
1:C:745:SER:O	1:C:748:LEU:HD23	0.43	2.13	3	1
1:B:695:LEU:HD23	1:B:695:LEU:O	0.43	2.13	4	1
1:C:755:LEU:O	1:C:755:LEU:HD22	0.43	2.12	5	1
1:B:742:ARG:O	1:B:746:ILE:HD12	0.43	2.14	8	1
1:B:679:LEU:O	1:B:683:ARG:N	0.43	2.51	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:708:VAL:HG21	1:C:744:ARG:HH22	0.43	1.73	12	1
1:A:755:LEU:C	1:A:755:LEU:HD23	0.43	2.34	7	2
1:B:755:LEU:HD21	1:C:706:ASN:HB3	0.43	1.89	9	1
1:A:704:LEU:O	1:A:704:LEU:HD13	0.43	2.12	13	1
1:B:775:LEU:O	1:B:775:LEU:HD23	0.43	2.12	1	1
1:C:689:VAL:O	1:C:692:LEU:CD1	0.43	2.67	5	1
1:C:771:LEU:CD2	1:C:775:LEU:HD23	0.43	2.43	7	1
1:C:771:LEU:H	1:C:771:LEU:HD13	0.43	1.74	10	1
1:A:715:LEU:HD22	1:A:715:LEU:H	0.43	1.74	7	1
1:A:763:LEU:HD22	1:A:763:LEU:H	0.43	1.74	9	1
1:B:693:ILE:HG21	1:C:689:VAL:CG1	0.43	2.43	13	1
1:C:712:TYR:CD2	1:C:713:SER:N	0.43	2.87	14	1
1:A:686:ILE:HG12	1:C:686:ILE:HG21	0.43	1.90	4	1
1:C:685:PHE:O	1:C:689:VAL:HG23	0.43	2.13	7	1
1:A:785:LEU:HD22	1:B:750:ASN:HD21	0.43	1.74	15	1
1:C:775:LEU:HD13	1:C:775:LEU:C	0.43	2.34	1	1
1:A:755:LEU:O	1:A:755:LEU:HD23	0.43	2.14	5	1
1:B:755:LEU:C	1:B:755:LEU:HD13	0.43	2.35	11	2
1:B:763:LEU:HD13	1:B:763:LEU:N	0.43	2.29	11	1
1:B:749:VAL:HG23	1:B:750:ASN:HD22	0.43	1.74	13	1
1:A:749:VAL:HG23	1:A:750:ASN:N	0.42	2.29	8	2
1:A:755:LEU:O	1:A:755:LEU:HD13	0.42	2.13	4	1
1:B:682:ILE:O	1:B:686:ILE:HD12	0.42	2.13	9	1
1:A:742:ARG:O	1:A:746:ILE:HD12	0.42	2.14	13	1
1:B:750:ASN:H	1:B:750:ASN:ND2	0.42	2.12	13	1
1:B:705:VAL:HG22	1:B:748:LEU:CD2	0.42	2.43	14	1
1:A:688:ILE:O	1:A:692:LEU:HD13	0.42	2.15	2	1
1:C:778:VAL:O	1:C:782:VAL:HG23	0.42	2.14	2	1
1:C:774:LEU:HD13	1:C:774:LEU:O	0.42	2.13	13	1
1:A:745:SER:O	1:A:748:LEU:HD23	0.42	2.13	15	1
1:A:763:LEU:O	1:A:774:LEU:HG	0.42	2.14	2	1
1:A:770:ARG:O	1:A:774:LEU:HD13	0.42	2.14	2	1
1:B:705:VAL:HG22	1:B:748:LEU:HD23	0.42	1.91	5	1
1:B:712:TYR:CG	1:B:713:SER:N	0.42	2.88	6	1
1:B:753:LEU:HD11	1:B:757:TRP:CZ3	0.42	2.50	10	1
1:A:758:ASP:OD2	1:B:715:LEU:HD11	0.42	2.15	5	1
1:A:764:SER:O	1:A:765:LEU:CB	0.42	2.66	7	1
1:A:701:VAL:O	1:A:705:VAL:HG23	0.42	2.14	10	2
1:C:750:ASN:H	1:C:750:ASN:ND2	0.42	2.12	12	1
1:B:775:LEU:HD13	1:B:775:LEU:C	0.42	2.34	15	1
1:C:684:ILE:HG13	1:C:687:ILE:HD11	0.42	1.90	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:765:LEU:HD23	1:C:765:LEU:O	0.42	2.15	14	1
1:B:743:ASP:O	1:B:746:ILE:HB	0.42	2.15	7	1
1:A:693:ILE:C	1:A:693:ILE:HD13	0.42	2.34	11	1
1:B:774:LEU:HD22	1:B:774:LEU:O	0.42	2.13	13	1
1:C:684:ILE:C	1:C:684:ILE:HD13	0.42	2.35	13	1
1:B:755:LEU:HD23	1:B:755:LEU:C	0.42	2.34	1	3
1:B:775:LEU:HD13	1:B:775:LEU:O	0.42	2.15	3	1
1:B:756:ILE:HD13	1:B:756:ILE:O	0.42	2.15	8	1
1:B:774:LEU:HD12	1:B:777:ILE:HD11	0.42	1.89	9	1
1:A:706:ASN:O	1:A:710:GLN:HB2	0.42	2.15	10	1
1:A:746:ILE:H	1:A:746:ILE:HD12	0.42	1.75	13	1
1:B:695:LEU:HD23	1:B:695:LEU:C	0.42	2.35	1	1
1:C:776:LEU:HD13	1:C:776:LEU:C	0.42	2.34	15	2
1:C:705:VAL:HG13	1:C:748:LEU:CD2	0.42	2.44	7	1
1:B:708:VAL:HG21	1:C:714:PRO:HD2	0.42	1.91	15	1
1:C:755:LEU:HD23	1:C:755:LEU:C	0.42	2.35	15	1
1:C:748:LEU:C	1:C:748:LEU:HD13	0.41	2.35	1	1
1:B:758:ASP:CB	1:C:710:GLN:HB3	0.41	2.45	3	1
1:A:763:LEU:HD22	1:A:763:LEU:N	0.41	2.30	5	1
1:C:713:SER:O	1:C:714:PRO:C	0.41	2.58	5	2
1:B:765:LEU:HD23	1:B:765:LEU:C	0.41	2.35	7	1
1:A:745:SER:O	1:A:748:LEU:HG	0.41	2.14	13	1
1:C:749:VAL:HG23	1:C:750:ASN:H	0.41	1.75	15	1
1:C:697:ILE:HD12	1:C:698:VAL:N	0.41	2.30	5	1
1:A:749:VAL:HG23	1:A:750:ASN:H	0.41	1.75	8	1
1:C:686:ILE:HD12	1:C:686:ILE:N	0.41	2.30	8	1
1:A:760:LEU:HD13	1:A:760:LEU:C	0.41	2.35	1	1
1:B:687:ILE:N	1:B:687:ILE:HD12	0.41	2.30	10	1
1:C:755:LEU:HD13	1:C:755:LEU:C	0.41	2.34	10	1
1:C:695:LEU:O	1:C:695:LEU:HD23	0.41	2.15	13	1
1:B:707:ARG:CZ	1:C:707:ARG:NH1	0.41	2.84	12	1
1:A:755:LEU:C	1:A:755:LEU:HD22	0.41	2.36	15	1
1:C:689:VAL:O	1:C:692:LEU:HD11	0.41	2.16	5	1
1:B:705:VAL:HG11	1:B:748:LEU:HD22	0.41	1.91	7	1
1:B:765:LEU:HD12	1:B:765:LEU:O	0.41	2.15	12	1
1:A:693:ILE:C	1:A:693:ILE:HD12	0.41	2.36	14	1
1:B:742:ARG:O	1:B:746:ILE:HG12	0.41	2.15	1	1
1:B:707:ARG:O	1:B:711:GLY:O	0.41	2.38	2	1
1:A:776:LEU:HD22	1:A:776:LEU:C	0.41	2.35	5	1
1:C:678:TRP:O	1:C:682:ILE:HD12	0.41	2.15	10	1
1:A:696:ARG:CG	1:C:693:ILE:HD11	0.41	2.46	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:683:ARG:HD2	1:A:683:ARG:C	0.41	2.36	3	1
1:C:755:LEU:C	1:C:755:LEU:HD23	0.41	2.36	6	2
1:A:692:LEU:HD23	1:C:693:ILE:HD12	0.41	1.91	9	1
1:C:771:LEU:N	1:C:771:LEU:HD23	0.41	2.31	12	1
1:C:706:ASN:O	1:C:710:GLN:CB	0.41	2.68	4	1
1:A:753:LEU:HD11	1:A:757:TRP:CZ3	0.41	2.51	10	1
1:C:680:TRP:HA	1:C:680:TRP:CE3	0.41	2.51	13	1
1:C:755:LEU:HD13	1:C:756:ILE:H	0.41	1.75	14	1
1:C:688:ILE:N	1:C:688:ILE:HD12	0.41	2.31	7	1
1:B:704:LEU:O	1:B:707:ARG:HB2	0.41	2.15	10	1
1:A:679:LEU:C	1:A:679:LEU:HD12	0.41	2.37	12	1
1:B:686:ILE:N	1:B:686:ILE:HD12	0.41	2.30	15	1
1:B:775:LEU:O	1:B:778:VAL:HG22	0.41	2.16	15	1
1:A:682:ILE:HD13	1:C:683:ARG:CZ	0.41	2.46	15	1
1:A:748:LEU:HD12	1:A:748:LEU:C	0.41	2.36	8	1
1:B:781:ILE:O	1:B:785:LEU:HD13	0.41	2.16	8	1
1:B:706:ASN:OD1	1:B:706:ASN:C	0.41	2.59	9	1
1:B:748:LEU:HD21	1:C:714:PRO:HG3	0.41	1.91	11	1
1:B:781:ILE:HG21	1:C:747:ARG:NH1	0.41	2.30	14	1
1:A:746:ILE:HG21	1:C:781:ILE:HD12	0.41	1.92	14	1
1:B:745:SER:O	1:B:748:LEU:HG	0.40	2.17	12	1
1:A:755:LEU:C	1:A:755:LEU:HD13	0.40	2.36	11	1
1:A:746:ILE:N	1:A:746:ILE:HD12	0.40	2.32	13	1
1:B:678:TRP:O	1:B:682:ILE:HD13	0.40	2.16	14	1
1:B:685:PHE:O	1:B:689:VAL:HG23	0.40	2.17	9	1
1:A:750:ASN:ND2	1:C:785:LEU:HD21	0.40	2.32	15	1
1:B:754:ALA:HB1	1:C:715:LEU:HD12	0.40	1.94	14	1
1:C:753:LEU:O	1:C:757:TRP:CB	0.40	2.70	7	1
1:A:763:LEU:H	1:A:763:LEU:HD13	0.40	1.75	9	1
1:C:763:LEU:CD1	1:C:763:LEU:H	0.40	2.30	15	1
1:B:678:TRP:CG	1:B:679:LEU:N	0.40	2.90	14	1
1:A:775:LEU:O	1:A:778:VAL:HG12	0.40	2.16	3	1
1:B:771:LEU:HD23	1:B:771:LEU:H	0.40	1.76	4	1
1:A:785:LEU:HD12	1:A:785:LEU:C	0.40	2.36	5	1
1:A:771:LEU:HD13	1:A:771:LEU:C	0.40	2.36	6	1
1:A:778:VAL:O	1:A:781:ILE:CG1	0.40	2.70	6	1
1:A:715:LEU:H	1:A:715:LEU:HD23	0.40	1.76	12	1
1:A:781:ILE:HD12	1:B:746:ILE:HG13	0.40	1.94	12	1
1:B:756:ILE:HG23	1:B:757:TRP:HE3	0.40	1.75	12	1
1:B:764:SER:CB	1:B:771:LEU:HD13	0.40	2.47	12	1
1:B:680:TRP:CH2	1:C:679:LEU:HD21	0.40	2.52	12	1

5.2 Torsion angles

5.2.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	85/112 (76%)	78±2 (91±2%)	5±1 (5±2%)	3±1 (3±2%)	7	39
1	B	86/112 (77%)	78±1 (91±1%)	4±1 (5±1%)	3±1 (4±1%)	5	31
1	C	86/112 (77%)	78±1 (91±1%)	4±1 (5±2%)	3±1 (4±2%)	5	31
All	All	3855/5040 (76%)	3516 (91%)	196 (5%)	143 (4%)	6	34

All 27 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	714	PRO	14
1	A	714	PRO	12
1	C	714	PRO	10
1	C	767	SER	8
1	C	769	HIS	8
1	C	765	LEU	8
1	B	767	SER	8
1	B	712	TYR	6
1	B	678	TRP	6
1	C	768	TYR	6
1	B	766	PHE	6
1	A	712	TYR	6
1	C	712	TYR	5
1	B	769	HIS	5
1	A	767	SER	4
1	B	765	LEU	4
1	C	766	PHE	4
1	A	768	TYR	3
1	A	766	PHE	3
1	A	741	ASP	3
1	A	765	LEU	3
1	A	769	HIS	3
1	B	711	GLY	2
1	C	711	GLY	2
1	A	711	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	B	768	TYR	1
1	A	715	LEU	1

5.2.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	81/101 (80%)	63±4 (78±5%)	18±4 (22±5%)	3	30
1	B	83/101 (82%)	65±3 (79±4%)	18±3 (21±4%)	3	31
1	C	83/101 (82%)	61±3 (74±3%)	22±3 (26±3%)	2	22
All	All	3705/4545 (82%)	2841 (77%)	864 (23%)	3	28

All 216 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	693	ILE	13
1	B	683	ARG	13
1	C	704	LEU	12
1	C	683	ARG	11
1	A	712	TYR	11
1	C	750	ASN	11
1	B	744	ARG	11
1	B	678	TRP	10
1	B	715	LEU	10
1	C	757	TRP	10
1	C	744	ARG	10
1	C	707	ARG	10
1	B	757	TRP	10
1	A	757	TRP	10
1	C	679	LEU	9
1	A	693	ILE	9
1	C	780	ARG	9
1	A	763	LEU	9
1	A	744	ARG	9
1	A	683	ARG	9
1	C	768	TYR	9

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Mol	Chain	Res	Type	Models (Total)
1	C	763	LEU	9
1	C	680	TRP	9
1	B	758	ASP	8
1	A	780	ARG	8
1	C	774	LEU	8
1	C	765	LEU	8
1	C	761	ARG	8
1	C	742	ARG	8
1	B	740	ARG	8
1	C	740	ARG	8
1	B	693	ILE	8
1	C	678	TRP	7
1	C	771	LEU	7
1	C	692	LEU	7
1	C	710	GLN	7
1	A	708	VAL	7
1	A	704	LEU	7
1	B	770	ARG	7
1	B	763	LEU	7
1	C	758	ASP	6
1	B	765	LEU	6
1	A	697	ILE	6
1	B	708	VAL	6
1	A	710	GLN	6
1	C	708	VAL	6
1	C	787	ARG	6
1	A	707	ARG	6
1	C	785	LEU	6
1	C	715	LEU	6
1	B	742	ARG	6
1	B	780	ARG	6
1	A	765	LEU	6
1	B	679	LEU	5
1	A	742	ARG	5
1	A	755	LEU	5
1	A	679	LEU	5
1	A	684	ILE	5
1	C	696	ARG	5
1	A	767	SER	5
1	A	709	ARG	5
1	B	713	SER	5
1	C	745	SER	5

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Mol	Chain	Res	Type	Models (Total)
1	B	704	LEU	5
1	A	713	SER	5
1	A	785	LEU	5
1	C	681	TYR	5
1	C	769	HIS	5
1	B	774	LEU	5
1	A	715	LEU	5
1	C	775	LEU	5
1	B	710	GLN	4
1	B	787	ARG	4
1	C	756	ILE	4
1	B	748	LEU	4
1	B	697	ILE	4
1	B	702	LEU	4
1	A	750	ASN	4
1	B	701	VAL	4
1	C	770	ARG	4
1	A	748	LEU	4
1	C	781	ILE	4
1	A	762	SER	4
1	A	768	TYR	4
1	B	766	PHE	4
1	C	766	PHE	4
1	A	753	LEU	4
1	A	740	ARG	4
1	B	750	ASN	4
1	A	771	LEU	4
1	A	761	ARG	4
1	C	788	ARG	4
1	A	766	PHE	4
1	A	686	ILE	4
1	B	707	ARG	4
1	C	685	PHE	4
1	A	781	ILE	3
1	A	706	ASN	3
1	B	681	TYR	3
1	C	747	ARG	3
1	A	741	ASP	3
1	C	677	ASN	3
1	B	695	LEU	3
1	A	739	GLU	3
1	A	773	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	764	SER	3
1	A	680	TRP	3
1	B	785	LEU	3
1	B	773	ASP	3
1	C	697	ILE	3
1	A	760	LEU	3
1	C	695	LEU	3
1	C	716	SER	3
1	B	783	GLU	3
1	B	769	HIS	3
1	A	747	ARG	3
1	C	709	ARG	3
1	A	770	ARG	3
1	C	755	LEU	3
1	A	783	GLU	3
1	B	684	ILE	3
1	A	774	LEU	3
1	A	691	SER	3
1	A	772	ARG	3
1	B	741	ASP	3
1	B	680	TRP	3
1	C	762	SER	3
1	B	747	ARG	3
1	C	741	ASP	3
1	A	681	TYR	3
1	B	760	LEU	3
1	B	761	ARG	3
1	B	753	LEU	3
1	C	784	LEU	3
1	B	768	TYR	3
1	B	691	SER	3
1	B	716	SER	3
1	C	748	LEU	2
1	A	756	ILE	2
1	A	745	SER	2
1	C	691	SER	2
1	A	759	ASP	2
1	A	685	PHE	2
1	B	687	ILE	2
1	A	752	SER	2
1	A	769	HIS	2
1	B	749	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	B	784	LEU	2
1	B	781	ILE	2
1	C	767	SER	2
1	B	788	ARG	2
1	B	745	SER	2
1	B	703	SER	2
1	A	758	ASP	2
1	C	702	LEU	2
1	B	755	LEU	2
1	B	771	LEU	2
1	A	743	ASP	2
1	A	695	LEU	2
1	B	709	ARG	2
1	B	772	ARG	2
1	C	777	ILE	2
1	A	702	LEU	2
1	B	777	ILE	2
1	A	775	LEU	2
1	B	756	ILE	2
1	B	779	THR	2
1	A	787	ARG	2
1	C	686	ILE	2
1	B	776	LEU	2
1	B	712	TYR	1
1	C	772	ARG	1
1	C	703	SER	1
1	B	682	ILE	1
1	C	749	VAL	1
1	B	699	PHE	1
1	C	712	TYR	1
1	A	776	LEU	1
1	C	682	ILE	1
1	C	739	GLU	1
1	A	698	VAL	1
1	C	701	VAL	1
1	B	698	VAL	1
1	C	753	LEU	1
1	C	698	VAL	1
1	C	713	SER	1
1	C	706	ASN	1
1	B	762	SER	1
1	A	778	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	C	689	VAL	1
1	C	684	ILE	1
1	B	677	ASN	1
1	A	788	ARG	1
1	B	688	ILE	1
1	A	692	LEU	1
1	A	716	SER	1
1	C	782	VAL	1
1	B	767	SER	1
1	C	778	VAL	1
1	B	692	LEU	1
1	B	759	ASP	1
1	A	782	VAL	1
1	B	778	VAL	1
1	B	686	ILE	1
1	B	743	ASP	1
1	C	779	THR	1
1	A	696	ARG	1
1	A	687	ILE	1
1	B	764	SER	1
1	C	773	ASP	1
1	B	696	ARG	1
1	B	739	GLU	1
1	C	746	ILE	1
1	A	689	VAL	1
1	A	688	ILE	1
1	B	706	ASN	1

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.4 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.5 Ligand geometry

There are no ligands in this entry.

5.6 Other polymers

There are no such molecules in this entry.

5.7 Polymer linkage issues

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 10% for the well-defined parts and 10% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *HIV-1_gp41_TMD-CTLLP2_chemical_shifts.tab*

6.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	460
Number of shifts mapped to atoms	460
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	106	-0.04 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	55	1.27 ± 0.07	Should be applied
$^{13}\text{C}'$	101	-0.15 ± 0.08	None needed (< 0.5 ppm)
^{15}N	99	0.58 ± 0.14	Should be applied

6.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 10%, i.e. 365 atoms were assigned a chemical shift out of a possible 3697. 0 out of 78 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	328/1334 (25%)	82/533 (15%)	164/536 (31%)	82/265 (31%)
Sidechain	37/2090 (2%)	0/1215 (0%)	37/738 (5%)	0/137 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/273 (0%)	0/141 (0%)	0/118 (0%)	0/14 (0%)
Overall	365/3697 (10%)	82/1889 (4%)	201/1392 (14%)	82/416 (20%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 367 atoms were assigned a chemical shift out of a possible 3729. 0 out of 78 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	330/1344 (25%)	82/537 (15%)	166/540 (31%)	82/267 (31%)
Sidechain	37/2100 (2%)	0/1221 (0%)	37/741 (5%)	0/138 (0%)
Aromatic	0/285 (0%)	0/147 (0%)	0/123 (0%)	0/15 (0%)
Overall	367/3729 (10%)	82/1905 (4%)	203/1404 (14%)	82/420 (20%)

6.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

6.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

